Supporting Information

Aromatic Interactions of Allenyl-anthracene Derivatives with π-electron Acceptor Molecules: an Experimental and Computational Study

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Computational methods

DFT in the Kohn−Sham formulation as implemented in Gaussian 09 (V. E.01.) [1] was used to locate minimum structures on the potential energy surfaces of the complexes under study. All calculations were done with the dispersion and long range corrected ωB97X-D density functional [2] of Jeng-Da Chai and Head-Gordon and coworkers in combination with the Ahlrich's split valence quality basis set including polarization functions def2SVP [3]. To achieve results with high accuracy, tight self-consistent field (SCF) criteria and an ultrafine pruned grid (99, 590) for the numerical integration were used. This consists of 99 radial shells and 590 angular points per shell. All calculations were performed in gas phase, and the stability of the wavefunction was checked for all stationary points found in this study [4]. Moreover, harmonic analysis of the second derivatives of the energy with respect to the nuclear displacements was performed to ensure that a minimum structure and not a transition state had been located. Interaction energies for the complexes under study were computed by means of the supermolecule method using the counterpoise procedure to avoid basis set superposition errors [5]. As the geometry of the molecules can change when the complex is formed, an additional contribution to the energy describing this effect (deformation energy) is also considered. Finally, the complexation energy of the system is obtained as a combination of the interaction and deformation energy terms.

Interaction energies were also computed by using the Symmetry Adapted Perturbation Theory approach (SAPT) [6,7]. This methodology provides a means of directly compute the noncovalent interaction energy in a complex and provides a decomposition of the global interaction in terms of four different components with physical meaning: electrostatic, exchange, induction and dispersion. Within the framework of Rayleigh-Schrödinger perturbation theory, the SAPT interaction energy of a complex can be written using a perturbative series expansion with respect to three different perturbation parameters, one describing the order with respect to the intermolecular potential and the other two designating the order with respect to the intramolecular electron correlation [6]. Because the SAPT interaction energy is based on a series expansion, this can be truncated according to the desired accuracy, being the SAPT0 level the simplest one. SAPT0 level is chosen to analyse the nature of the intermolecular interaction not only because the existence of a well balance between the accuracy of results and the computational cost

associated with the calculation, but also for being the only SAPT approach for which the partition of energies in terms of fragments and functional groups (F-SAPT0) is available [8-11] .

All calculations related to the SAPT methodology have been carried out with the PSI4 1.1 software [12], benefiting from the density-fitting approach. This procedure introduces negligible errors into the SAPT energy and greatly improves the computational efficiency. In all cases, jun-cc-pVDZ basis set was used as recommended by Trent M. Parker and coworkers [7]. Jun-cc-pVDZ basis [13] set is created removing diffuse functions (diffuse from H and He and also the highest angular momentum diffuse function from the rest of the atoms) from the well-known Dunning's correlation consistent basis set: aug-cc-pVDZ. To make use of the density fitting approach the corresponding auxiliary basis (jun-cc-pVDZ-ri and jun-cc-pVDZ-jkfit) were employed. The different terms of the SAPT0 energy equation are grouped according to their nature (electrostatic, repulsion, induction, and dispersion) following the proposal of Parker et al. [7]. In all cases δ_{HF} correction that is used to take into account higher-order induction effects and is always included in the induction term.

The computational study of the complexes is complemented by using two different electron density analysis: Quantum Theory of Atoms in Molecules (QTAIM) [14-15] and Non-Covalent interaction analysis (NCI) [16], using for this purpose in both cases the Multiwfn program [17].

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Complexes $(MEA)_2A:X$ (X = 1-4)

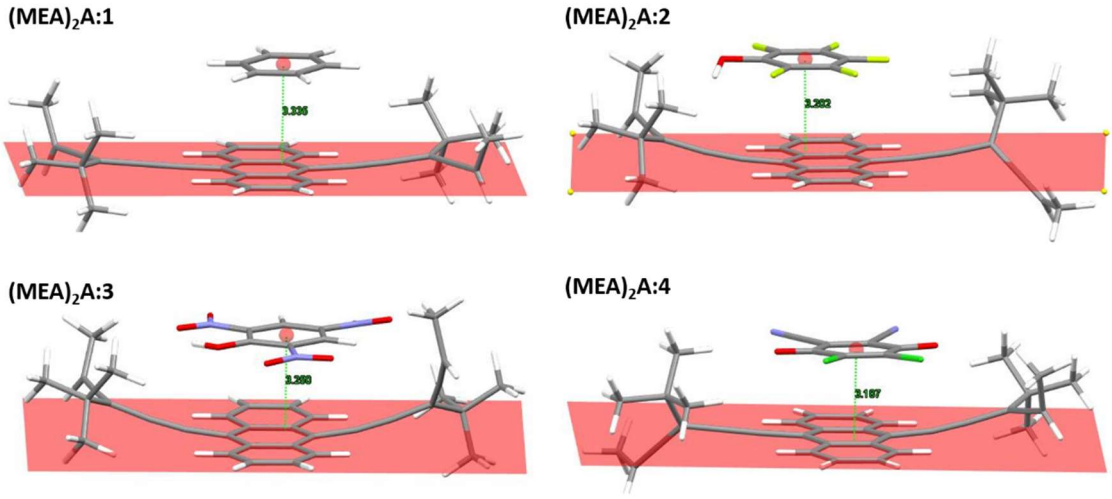

Figure S1. Intermolecular distances in complexes **$(MEA)_2A:X$** (X = 1-4).

Table S1. Electronic energies ($E_{SCF,298}$), free (G_{298}), and enthalpies (H_{298}) energies for all conformers of complexes **$(MEA)_2A:X$** (X = 1-4) (in Hartree) computed at wB97X-D/def2-SVP level. Note that the filenames are used in our calculations and do not follow any guide. These energies are similar for the complexes involving the enantiomer *P,P* allenyl-anthracene.

Filename	$E_{SCF,298}$ wB97X-D/def2-SVP	G_{298} wB97X-D/def2-SVP	H_{298} wB97X-D/def2-SVP
antra_01	-1314.5507389	-1314.0459430	-1313.9405580
antra_02	-1314.5507500	-1314.0459720	-1313.9405570
benzene	-232.0014242	-231.9273600	-231.8946240
Pentafluorophenol	-802.7663272	-802.7368390	-802.6902480
Picric acid	-919.9773005	-919.9020140	-919.8478770
DDQ	-1484.1855979	-1484.1613050	-1484.1079870
$(MEA)_2A:1$			
antra_benz_02	-1546.5691471	-1545.9740460	-1545.8504390

antra_benz_05	-1546.5691471	-1545.9738700	-1545.8504420
antra_benz_03	-1546.5691472	-1545.9738040	-1545.8504420
antra_benz_01	-1546.5694954	-1545.9723610	-1545.8506970
antra_benz_07	-1546.5694955	-1545.9722740	-1545.8506930
antra_benz_04	-1546.5694960	-1545.9722270	-1545.8506820
antra_benz_08	-1546.5695165	-1545.9715050	-1545.8507140
$(MEA)_2A$:2			
antra_pF_02	-2117.3514010	-2116.7945110	-2116.6631020
antra_pF_09	-2117.3513744	-2116.7935460	-2116.6629120
antra_pF_01	-2117.3513100	-2116.7928800	-2116.6627800
antra_pF_10	-2117.3508011	-2116.7932820	-2116.6623520
antra_pF_04	-2117.3505721	-2116.7932550	-2116.6619740
antra_pF_07	-2117.3504524	-2116.7933280	-2116.6621260
antra_pF_05	-2117.3501124	-2116.7913550	-2116.6614880
antra_pF_08	-2117.3491959	-2116.7910970	-2116.6606130
antra_pF_03	-2117.3485344	-2116.7918720	-2116.6599170
$(MEA)_2A$:3			
antra_picric_06	-2234.5767277	-2233.9689130	-2233.8350470
antra_picric_08	-2234.5767050	-2233.9690040	-2233.8347710
antra_picric_07	-2234.5748394	-2233.9669800	-2233.8330770
antra_picric_02	-2234.5745793	-2233.9678320	-2233.8327740
antra_picric_04	-2234.5727870	-2233.9675780	-2233.8312140
antra_picric_09	-2234.5727870	-2233.9675670	-2233.8312140
antra_picric_05	-2234.5723299	-2233.9662380	-2233.8308800
antra_picric_10	-2234.5721651	-2233.9648380	-2233.8304520
antra_picric_11	-2234.5721651	-2233.9648270	-2233.8304480
antra_picric_03	-2234.5720544	-2233.9677190	-2233.8304150
$(MEA)_2A$:4			
antra_ddq_06	-2798.7808616	-2798.2248470	-2798.0910400
antra_ddq_09	-2798.7806929	-2798.2238850	-2798.0905340
antra_ddq_10	-2798.7806929	-2798.2237860	-2798.0905290
antra_dd1_01	-2798.7797665	-2798.2252110	-2798.0898110
antra_ddq_04	-2798.7794149	-2798.2237670	-2798.0893630

antra_ddq_03	-2798.7792012	-2798.2229190	-2798.0892640
antra_ddq_02	-2798.7789923	-2798.2245200	-2798.0891000
antra_ddq_08	-2798.7781197	-2798.2231080	-2798.0880320
antra_ddq_07	-2798.7779881	-2798.2237930	-2798.0881240

Experimental part

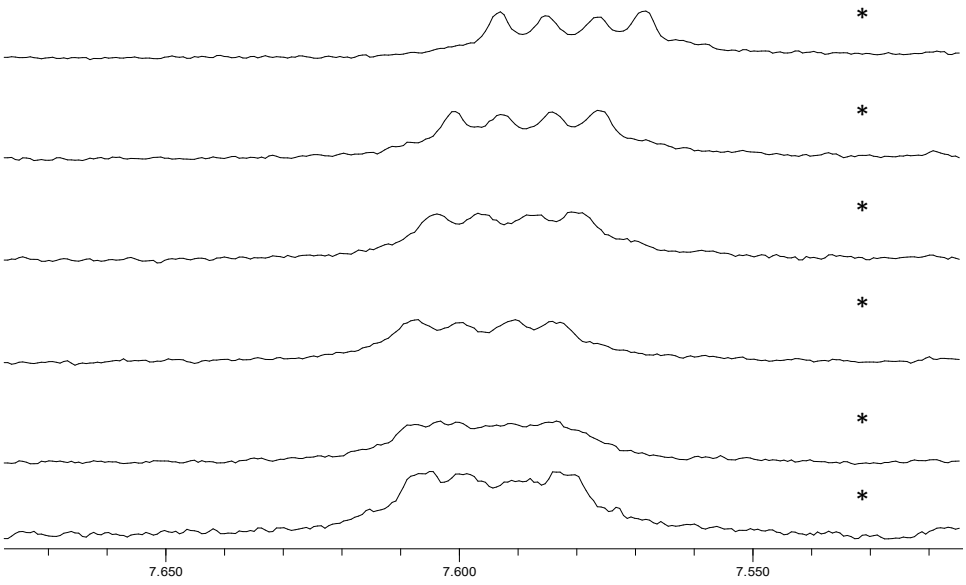

Figure S2. ^{1}H NMR of: ***(DEA)$_2$A** and ****(DEA)$_2$A** upon addition of DDQ in chloroform.

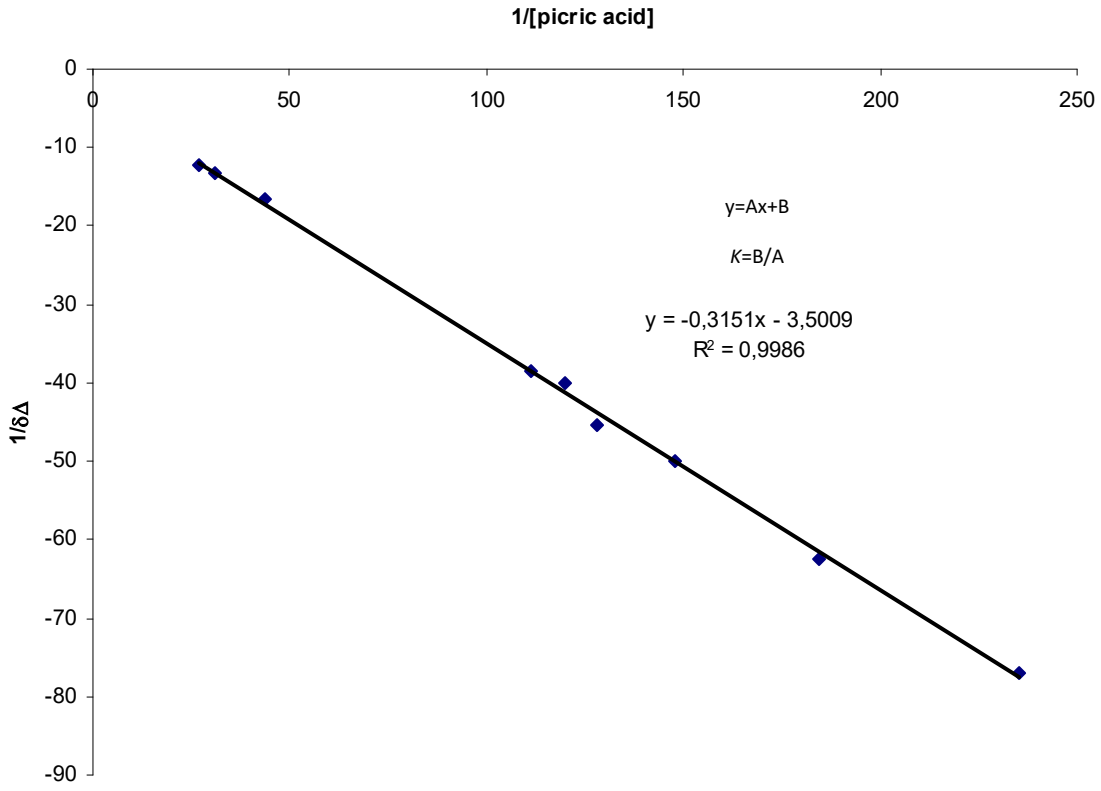

Figure S3. Benesi-Hildebrand plot for **$(DEA)_2A_4$** with picric acid.

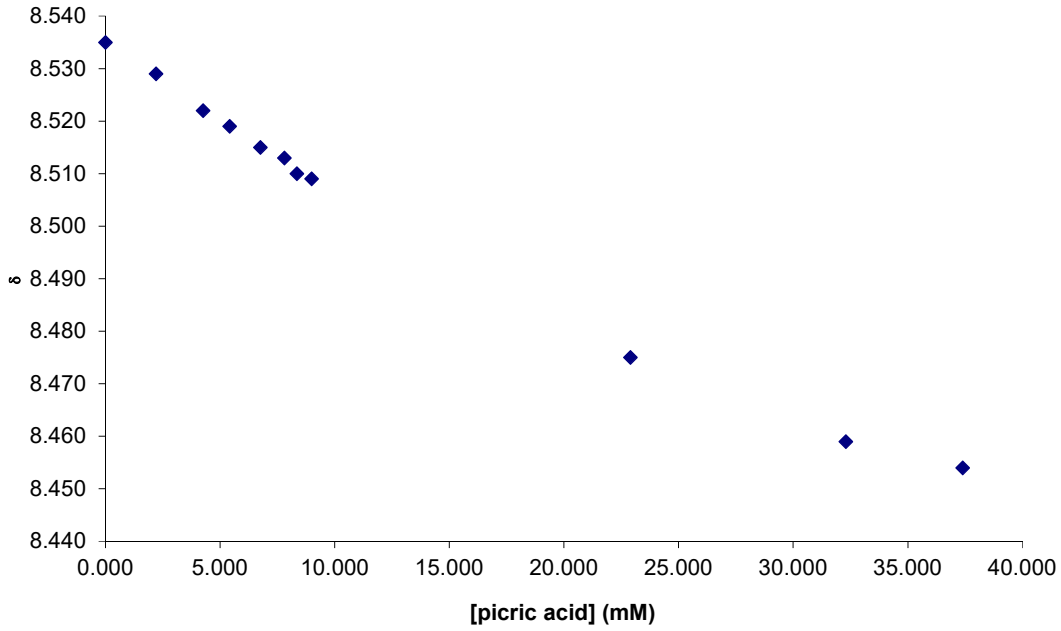

Figure S4 Study of association between **$(DEA)_2A_4$** and picric acid.

SAPT0 and F-SAPT0

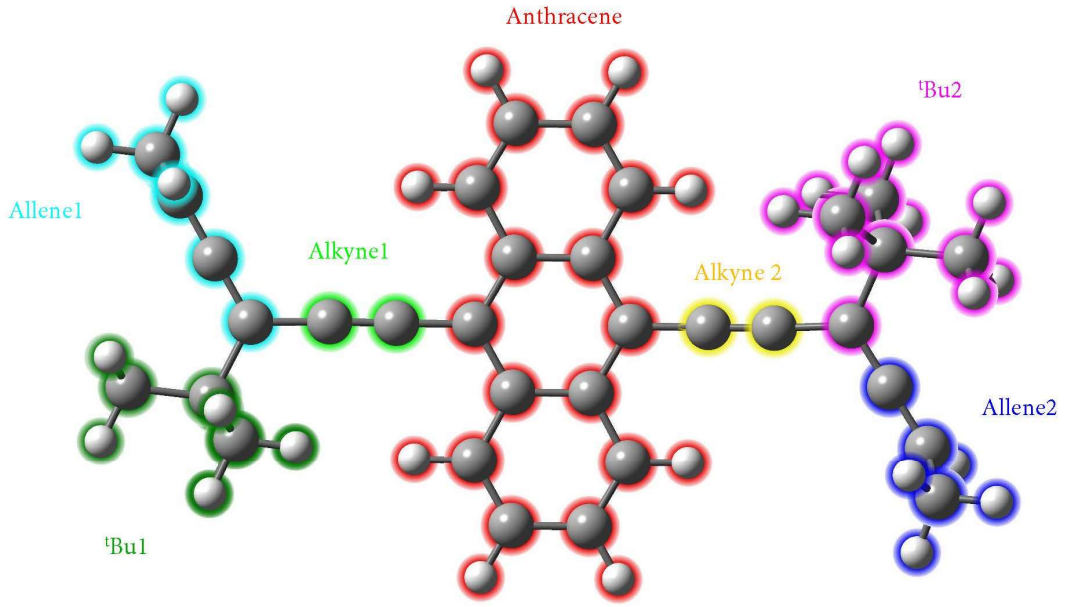

Figure S5. Highlighted fragments in which the heterooligomer was divided

System $(MEA)_2A$:1

Among all the fragments defined in the oligomer, the one that has a more substantial contribution is the anthracene ring. This interaction represents the 55.48% of the global interaction energy that is -25,5 kJ/mol. The benzene-anthracene interaction is largely dominated by the dispersive component since it contributes more than 75% of the global. The alkyne groups that bind the chiral part of the oligomer with the anthracene ring also have a significant contribution. The spatial arrangement of minimum energy analysed locates the benzene ring slightly displaced towards one of the alkyne groups, making the repulsive interaction with this moiety higher. Although there is a greater contribution of repulsion, the rest of interactions compensate that value and allow the alkyne fragment to contribute a 14.62% to the global interaction energy. The alkyne group on the opposite side has a practically zero repulsion contribution which allows this moiety to have a greater interaction energy (17.93% of the total) although the value of dispersion come down and the induction contribution slightly destabilizes the system (0.2 kJ/mol). The displacement of the position of the benzene molecule with respect to the central axis of the

anthracene favours the system to stablish a favourable interaction with one of the tBu groups that substitute the allene moiety. Therefore, significantly higher interaction energies are obtained with that tBu group compared with the rest of the fragments not analysed before. More specifically, numerically this tBu group contributes 7.62% to the global interaction energy thanks mainly to the high value of the dispersion term that represents, (as it did with the anthracene group), more than 75% of the global interaction energy. The remaining 4.35% of the interaction energy is given by the contributions of the simplified allene located in the region closest to the benzene ring and by the tBu group and the allene on the opposite side. It should be noted that although they represent a low amount of the interaction energy, both have a positive electrostatic contribution that destabilize the system. The results of the F-SAPT0 analysis can be found on table S2.

Based on this study, it can be concluded that most of the favourable interaction between benzene and oligomer is given by the anthracene fragment thanks to the existence of strong dispersive interactions followed by the alkyne-type connectors whose global contribution is around 32.50 % of the global. The slight displacement of the benzene molecule makes it possible to establish stabilizing interactions between one of the tBu groups and the guest, representing a 7.62% of the global. It is expected that in the other systems a very significant contribution to the global energy of the anthracene is obtained due to the establishment of predominantly dispersive aromatic interactions as it happens in this simple system, however, the existence of diverse functional groups replacing the benzene core it can allow to establish other types of interactions with the lateral groups that are not possible due to the small size of the benzene core.

System $(MEA)_2A$:2

Again, the anthracene core has the greatest contribution to interaction energy (54.96%) that numerically corresponds to more than -42.0 kJ/mol of a total interaction energy of -70,567 kJ/mol. This interaction is clearly dominated by the dispersion component since it represents approximately a 62.00 % of the stabilizing energy components. The substitution of all hydrogen atoms of the benzene core by five fluorine atoms and a hydroxyl group modifies the nature of the interaction of the pi-electron acceptor molecule with the oligomer, increasing the relevance of the electrostatic component by more than 14%. While in the system bearing benzene the electrostatic component represented the 17.79% of the anthracene-benzene interaction, in this case the percentage increases up to the 32.26%. The interaction between the pentafluorophenol molecule (PFF) with one of the alkyne groups is the second one that has a greater relevance in the stabilization of the complex and represents the 31.22% of the overall interaction. This interaction is dominated by the electrostatic component due to the existence of a contact between the oxygen atom of the hydroxyl group of PFF and the π electronic density of the alkyne group. The

orientation of the pentafluorophenol molecule plays a very important role in the stabilization of pentafluorophenol in the oligomer surface. If the molecule is rotated and placed in another position, the stabilizing interaction provided by the hydroxyl group is loss making the stabilizing interaction energy of this group to decrease. It should be noted that, contrary to what happens with the benzene molecule, the second alkyne group destabilizes the system due to the existence of a positive electrostatic component of +5.8 kJ/mol. The high positive electrostatic component value in combination with a positive induction term cause a negative overall balance in the sense of destabilizing the global complex by +3.3 kJ/mol. The positive electrostatic interaction arise from a non-optimum orientation of multipole moments between the PFF molecule and the alkyne fragment.

The spatial arrangement of the pentafluorophenol molecule makes the hydroxyl group to interact with one of the alkyne moieties. This orientation makes the fluorine atom located opposite to the OH group to be orientated in such a way that is able to establish a stabilizing interaction with one of the tBu groups. This contact can also be visualized with a topological study of the electronic density. The AIM methodology reveals the existence of two hydrogen bonds between the fluorine atom opposite to the hydroxyl group and two hydrogen atoms of the tBu group. The distances of these contacts are 2.663 Å and 2.654 Å. The PFF-tBu contact represents the 4.82% of the global interaction energy. Numerically the contribution is -3.7 kJ/mol and is dominated by the dispersive component (67.54%) followed by induction and dispersion with an importance of the 28.13% and 4.33% respectively.

Table S2: Individual values of the different energetic components (in kJ/mol) of the global interaction energy obtained with the F-SAPT0 methodology for each of the four systems analysed in this study.

Molecule	Fragment	Electrostatic	Exchange	Induction	Dispersion	Total
Benzene	Anthracene	-14.760	57.475	-5.764	-62.424	-25.473
Benzene	Alkyne 1	-5.325	7.415	-0.690	-8.118	-6.713
Benzene	Alkyne 2	-5.325	0.443	0.150	-3.499	-8.230
Benzene	Allene 1	0.163	0.004	0.013	-0.481	-0.301
Benzene	tBu1	0.054	0.004	0.109	-0.627	-0.460
Benzene	Allene 2	-0.284	0.008	-0.008	-0.953	-1.237
Benzene	tBu2	-1.743	3.561	-0.017	-5.300	-3.499
Benzene	All	-27.216	68.916	-6.207	-81.406	-45.913

Molecule	Fragment	Electrostatic	Exchange	Induction	Dispersion	Total
DDQ	Anthracene	-84.904	125.375	-35.576	-117.851	-112.960
DDQ	Alkyne 1	12.624	7.123	-2.842	-11.453	5.447
DDQ	Alkyne 2	3.674	15.984	-4.924	-14.580	0.159

DDQ	Allene 1	-1.601	0.025	-0.263	-1.020	-2.859
DDQ	tBu1	-3.482	11.742	-0.932	-10.784	-3.461
DDQ	Allene 2	-2.149	2.312	-0.610	-5.986	-6.429
DDQ	tBu2	-0.686	4.360	-0.276	-6.458	-3.051
DDQ	All	-76.523	166.924	-45.424	-168.128	-123.151

Molecule	Fragment	Electrostatic	Exchange	Induction	Dispersion	Total
PFF	Anthracene	-37.277	73.125	-6.763	-71.495	-42.410
PFF	Alkyne 1	-23.433	18.145	-4.376	-14.429	-24.094
PFF	Alkyne 2	5.773	1.509	-0.021	-3.958	3.302
PFF	Allene 1	0.961	7.386	-1.735	-7.127	-0.510
PFF	tBu1	0.347	3.591	-2.253	-5.409	-3.720
PFF	Allene 2	-1.170	0.004	-0.013	-0.347	-1.526
PFF	tBu2	-1.237	4.636	-0.134	-4.874	-1.609
PFF	All	-56.037	108.400	-15.295	-107.639	-70.567

Molecule	Fragment	Electrostatic	Exchange	Induction	Dispersion	Total
Picric Ac.	Anthracene	-51.381	88.670	-16.072	-100.153	-78.939
Picric Ac.	Alkyne 1	-7.386	13.192	-2.149	-12.732	-9.079
Picric Ac.	Alkyne 2	-10.956	14.392	-3.302	-17.397	-17.263
Picric Ac.	Allene 1	-0.853	5.430	-0.573	-6.517	-2.508
Picric Ac.	tBu1	-0.857	2.663	-0.393	-5.835	-4.418
Picric Ac.	Allene 2	-3.691	9.041	-1.041	-12.544	-8.239
Picric Ac.	tBu2	-1.070	8.134	-0.732	-7.871	-1.542
Picric Ac.	All	-76.193	141.522	-24.265	-163.053	-121.989

Table S3: Details of the interaction energy components obtained after further decomposition of DDQ and picric acid into fragments considering the Allenyl-anthracene derivative as a single moiety.

Fragment Picric ac.	Fragment	Electrostatic	Exchange	Induction	Dispersion	Total
Ring	All	-16.745	59.243	12.632	-70.575	-15.445
Nitro (C4)	All	-12.686	18.158	-11.232	-24.102	-29.858
Nitro (C5)	All	-17.000	22.660	-10.575	-25.164	-30.083
Nitro (C10)	All	-23.061	24.787	-10.559	-24.804	-33.636
OHC2	All	-6.090	11.474	-2.558	-13.188	-10.362
H11	All	-0.238	3.361	-0.936	-3.269	-1.083
H14	All	-0.376	1.843	-1.041	-1.952	-1.526

Fragment DDQ	Fragment	Electrostatic	Exchange	Induction	Dispersion	Total
Ring + CO	All	-33.018	97.068	2.859	-98.527	-31.618

CN (C1)	All	-11.261	22.484	-16.202	-23.103	-28.085
CN (C2)	All	-13.690	25.820	-16.825	-24.415	-29.110
Cl (C7)	All	-9.087	11.671	-7.616	-10.743	-15.771
Cl (C10)	All	-9.468	9.886	-7.641	-11.345	-18.568

Cartesian Coordinates

$(MEA)_2A$

SCF = -1314.55073892

Num. Imaginary Freq = 0

C	0.711114	3.591984	-0.021968
C	1.399135	2.411891	-0.043419
C	0.715456	1.155150	-0.021976
C	-0.715620	1.155097	0.022379
C	-1.399354	2.411797	0.043897
C	-0.711398	3.591931	0.022540
C	1.419534	-0.073049	-0.043667
C	-1.419595	-0.073176	0.044043
C	-0.715824	-1.301577	0.022459
C	0.715880	-1.301521	-0.021959
C	1.401229	-2.557475	-0.043468
H	2.491879	-2.552878	-0.077973
C	0.711511	-3.736420	-0.021938
C	-0.711292	-3.736479	0.022708
C	-1.401093	-2.557581	0.044093
H	1.252351	4.540237	-0.038978
H	2.489555	2.407766	-0.077654
H	-2.489772	2.407643	0.078151
H	-1.252706	4.540143	0.039650
H	1.252067	-4.685155	-0.039061
H	-1.251763	-4.685259	0.039949
H	-2.491743	-2.553032	0.078589
C	-2.846052	-0.072661	0.087297
C	2.845990	-0.072440	-0.087098
C	-5.494433	-0.057912	0.165233
C	5.494629	-0.057733	-0.165537
C	6.153768	-1.203019	-0.183233
C	-6.153835	-1.203056	0.182931
C	-6.802643	-2.338339	0.186688
H	-7.030631	-2.794397	1.159611
C	6.802180	-2.338531	-0.187252
H	7.029781	-2.794488	-1.160317
C	7.266085	-3.073909	1.041234
H	6.828695	-4.083926	1.076221
H	8.360934	-3.193103	1.030574
H	6.982317	-2.540523	1.958454

C	-6.185806	1.318171	0.187778
C	-5.781983	2.089981	-1.078383
H	-6.240509	3.091281	-1.077507
H	-4.690436	2.214179	-1.141891
H	-6.114101	1.560234	-1.984179
C	-7.706956	1.154555	0.225064
H	-8.029659	0.603961	1.121421
H	-8.190407	2.143341	0.238531
H	-8.073000	0.607276	-0.656826
C	-5.718350	2.082676	1.436326
H	-6.176851	3.083585	1.465096
H	-6.003204	1.547102	2.354629
H	-4.625009	2.207486	1.444287
C	6.186086	1.318238	-0.188114
C	5.782959	2.089755	1.078466
H	6.241524	3.091039	1.077630
H	4.691446	2.214005	1.142541
H	6.115494	1.559742	1.983951

Benzene 1

SCF = -232.001424239

Num. Imaginary Freq = 0

C	-1.161422	-0.772615	-0.000001
C	0.088508	-1.392097	0.000114
C	1.249819	-0.619506	-0.000087
C	1.161356	0.772708	0.000019
C	-0.088391	1.392101	0.000081
C	-1.249871	0.619411	-0.000084
H	-2.070544	-1.377565	-0.000069
H	0.157646	-2.481915	0.000057
H	2.228304	-1.104294	-0.000192
H	2.070619	1.377434	-0.000011
H	-0.157771	2.481895	0.000043
H	-2.228250	1.104432	-0.000076

Pentafluorophenol 2

SCF = -802.766327242

Num. Imaginary Freq = 0

C	1.317769	-0.497261	-0.000025
C	0.236789	-1.375728	0.000025
C	-1.057868	-0.867253	-0.000033
C	-1.308858	0.506687	0.000025
C	-0.214231	1.376921	-0.000029
C	1.086646	0.878125	0.000026
O	-2.552749	1.007056	0.000021
H	-3.185706	0.279683	0.000063
F	-0.414534	2.683728	-0.000025
F	-2.106947	-1.692861	-0.000019
F	0.439314	-2.681202	0.000020
F	2.555200	-0.963711	-0.000020
F	2.109880	1.713481	0.000026

Num. Imaginary Freq = 0

Picric acid 3

SCF = -919.977300523

Num. Imaginary Freq = 0

C	1.545573	-0.033272	0.021544
C	0.886406	1.192636	-0.003522
C	-0.493591	1.214617	-0.005856
C	-1.274399	0.031624	-0.024091
C	-0.541581	-1.186989	-0.010662
C	0.847784	-1.225187	0.018797
H	1.450121	2.125538	-0.022359
H	1.370453	-2.181149	0.032607
O	-2.576603	0.097632	-0.082497
H	-2.918537	-0.826995	-0.111418
N	-1.143865	2.535633	0.014935
O	-2.165306	2.642614	0.647459
O	-0.577206	3.423355	-0.582591
N	-1.246313	-2.466339	-0.035160
O	-0.604037	-3.480302	0.004560
O	-2.473049	-2.435631	-0.096419
N	3.016070	-0.060382	0.043628
O	3.547650	-1.146717	0.055118
O	3.585497	1.006504	0.049381

DDQ 4

SCF = -1484.18559788

C	0.116433	-1.462651	-0.000030
C	-1.158143	-0.675473	0.000009
C	-1.158142	0.675473	-0.000010
C	0.116442	1.462652	0.000018
C	1.400912	0.676342	0.000021
C	1.400908	-0.676343	-0.000020
O	0.134055	2.662938	-0.000037
O	0.134050	-2.662934	0.000002
Cl	-2.589509	1.604235	-0.000049
Cl	-2.589516	-1.604230	0.000061
C	2.610635	1.442315	0.000049
N	3.590043	2.056257	0.000096
C	2.610627	-1.442323	-0.000038
N	3.590033	-2.056268	-0.000082

$(MEA)_2A$:1

SCF = -1546.56951651

Num. Imaginary Freq = 0

C	-0.761584	-3.382594	1.235733
C	-1.470942	-2.227565	1.063893
C	-0.807725	-0.968154	0.926219
C	0.622046	-0.938323	0.967619
C	1.327366	-2.168472	1.151280

C	0.660195	-3.352649	1.283309	H	-7.207715	-2.464032	1.576332
C	-1.529324	0.230486	0.718306	C	-7.139605	-3.111940	-0.558088
C	1.304704	0.289023	0.801887	H	-6.688210	-4.097583	-0.364467
C	0.582907	1.491926	0.619201	H	-8.224083	-3.267005	-0.671478
C	-0.846720	1.461907	0.574757	H	-6.741552	-2.727731	-1.506947
C	-1.549640	2.687833	0.353593	C	6.006630	-1.164929	0.473544
H	-2.639954	2.662078	0.322238	C	5.370843	-1.958904	-0.679108
C	-0.879036	3.866194	0.182959	H	5.792560	-2.975392	-0.720423
C	0.543282	3.894883	0.226092	H	4.280825	-2.044481	-0.553865
C	1.249284	2.744346	0.439023	H	5.562928	-1.468887	-1.646233
H	-1.286322	-4.334764	1.339558	C	7.517180	-1.059400	0.252738
H	-2.561364	-2.246644	1.026771	H	8.002932	-0.494818	1.062627
H	2.417228	-2.140356	1.179000	H	7.963285	-2.065205	0.221970
H	1.217397	-4.281495	1.422079	H	7.748783	-0.553585	-0.696905
H	-1.434380	4.791160	0.013865	C	5.728211	-1.872516	1.809044
H	1.069689	4.841883	0.089589	H	6.144151	-2.892166	1.796001
H	2.339975	2.760619	0.472221	H	6.185638	-1.324509	2.646607
C	2.729919	0.302318	0.757962	H	4.647967	-1.946672	2.005205
C	-2.951184	0.190896	0.608829	C	-6.291373	1.458779	0.042330
C	5.366214	0.235460	0.517085	C	-6.014142	2.431951	1.198985
C	-5.586724	0.122960	0.343826	H	-6.481965	3.408332	0.997293
C	-6.228127	-1.025726	0.468425	H	-6.421121	2.044006	2.145064
C	6.059677	1.355860	0.417115	H	-4.934284	2.592551	1.337367
C	6.740262	2.466458	0.302571	C	-7.800375	1.249700	-0.103010
H	7.118707	2.932644	1.222317	H	-8.293265	2.210064	-0.318335
C	-6.856200	-2.167304	0.578868	H	-8.031653	0.555266	-0.924911

H	-8.239274	0.839288	0.818752
C	-5.721826	2.028566	-1.266530
H	-6.190390	2.998338	-1.496353
H	-4.634387	2.182615	-1.197347
H	-5.913434	1.345990	-2.108505
C	3.941641	0.303097	0.662854
C	-4.160468	0.141762	0.492580
C	7.050007	3.160385	-0.996621
H	6.647609	4.185460	-0.993846
H	8.138678	3.238262	-1.144058
H	6.620494	2.620707	-1.851429
C	1.984638	-0.713719	-2.446204
C	0.994436	0.265957	-2.527233
C	1.627192	-2.055101	-2.318320
C	-0.351108	-0.096366	-2.483609
C	0.280501	-2.418078	-2.271392
C	-0.707943	-1.439056	-2.355056
H	1.272675	1.319434	-2.604744
H	3.038474	-0.427310	-2.461750
H	2.402161	-2.821863	-2.244485
H	0.000772	-3.467186	-2.152975
H	-1.762332	-1.719099	-2.299022
H	-1.125778	0.672392	-2.529525

$(MEA)_2A$:2

SCF = -2117.35131003

Num. Imaginary Freq = 0

C	0.640725	-2.441716	-2.531649
C	1.267264	-1.302231	-2.112157
C	0.519152	-0.196068	-1.598669
C	-0.906623	-0.303075	-1.532780
C	-1.524868	-1.510681	-1.985988
C	-0.776701	-2.547142	-2.467711
C	1.155206	0.967615	-1.103246
C	-1.666275	0.753358	-0.976282
C	-1.030648	1.931793	-0.520063
C	0.394735	2.039340	-0.582246
C	1.017124	3.223089	-0.075464
H	2.104643	3.298518	-0.122635
C	0.272297	4.237719	0.454111
C	-1.146150	4.131128	0.515674
C	-1.775368	3.013669	0.046385
H	1.229665	-3.280733	-2.906864
H	2.355288	-1.225450	-2.145629
H	-2.611477	-1.588617	-1.929002
H	-1.265732	-3.465540	-2.797663
H	0.763992	5.135349	0.834709
H	-1.730872	4.947501	0.944529
H	-2.861402	2.923264	0.097140
C	-3.077018	0.600429	-0.814390
C	2.578703	1.005459	-1.033404

C	-5.649761	0.198056	-0.329514	C	5.781831	3.186706	-0.648236
C	5.185806	0.759190	-0.648867	H	6.289212	4.000796	-0.107670
C	5.713830	-0.401107	-0.999713	H	6.222709	3.114370	-1.653930
C	-6.578693	0.966587	-0.867516	H	4.722173	3.461569	-0.762840
C	-7.497711	1.734994	-1.391829	C	7.417296	1.506797	0.247078
H	-7.917535	1.440840	-2.363033	H	7.947540	2.298891	0.797434
C	6.153089	-1.591387	-1.313392	H	7.555686	0.560814	0.791932
H	6.623240	-1.727680	-2.296305	H	7.890914	1.399169	-0.740287
C	6.041104	-2.795151	-0.415417	C	5.306073	1.989135	1.512091
H	5.563524	-3.626011	-0.956760	H	5.783121	2.802781	2.080112
H	7.037259	-3.140168	-0.096291	H	4.228707	2.210974	1.451687
H	5.432388	-2.571456	0.470219	H	5.440865	1.058685	2.087698
C	-5.957298	-0.968604	0.629260	C	-4.267411	0.449844	-0.624827
C	-5.293750	-0.670027	1.983806	C	3.785803	0.938681	-0.902981
H	-5.472974	-1.500148	2.685087	C	-8.028017	2.997371	-0.767587
H	-4.206475	-0.544497	1.877891	H	-7.859404	3.858709	-1.432769
H	-5.705909	0.249414	2.427312	H	-9.114172	2.921113	-0.601886
C	-7.468022	-1.123599	0.815448	H	-7.542521	3.202209	0.196177
H	-7.970776	-1.337921	-0.139783	C	-0.704500	-1.738872	1.342622
H	-7.676877	-1.954734	1.506237	C	-0.185710	-0.536506	1.815560
H	-7.916629	-0.210448	1.235218	C	0.155962	-2.733067	0.886662
C	-5.371459	-2.261096	0.039008	C	1.191839	-0.346019	1.830867
H	-5.580985	-3.111629	0.706305	C	1.532712	-2.527207	0.900982
H	-5.812676	-2.480267	-0.945622	C	2.073251	-1.333198	1.381811
H	-4.280337	-2.187037	-0.075804	O	3.406250	-1.174202	1.398446
C	5.935235	1.862239	0.113896	H	3.620861	-0.232971	1.353360

F	-2.015210	-1.926331	1.300017
F	-0.335489	-3.865514	0.413154
F	2.336784	-3.468033	0.429446
F	1.700558	0.810436	2.253327
F	-0.999236	0.415583	2.239184

$(MEA)_2A$:3

SCF = -2234.57216511

Num. Imaginary Freq = 0

C	-0.560519	4.046373	-1.402571
C	-1.256266	2.875195	-1.503479
C	-0.573132	1.622277	-1.598989
C	0.858713	1.617548	-1.586161
C	1.549104	2.864772	-1.484087
C	0.862533	4.041685	-1.397674
C	-1.277521	0.395138	-1.641760
C	1.555084	0.386907	-1.611494
C	0.850936	-0.837552	-1.716960
C	-0.579971	-0.831893	-1.734931
C	-1.271131	-2.083624	-1.762414
H	-2.361805	-2.075518	-1.765351
C	-0.589254	-3.267400	-1.755579
C	0.833668	-3.273273	-1.735578
C	1.529835	-2.096996	-1.725482
H	-1.097556	4.992814	-1.317751
H	-2.347071	2.873991	-1.496290
H	2.639920	2.853553	-1.466868
H	1.404620	4.985026	-1.310361
H	-1.137500	-4.211185	-1.757892
H	1.371397	-4.223285	-1.726950
H	2.621118	-2.101631	-1.708936
C	2.962863	0.351514	-1.395711
C	-2.687506	0.382459	-1.429736
C	5.459588	0.030356	-0.583588
C	-5.185374	0.344768	-0.551774
C	-5.423624	1.190650	0.435184
C	5.909681	-1.211852	-0.549068
C	6.278849	-2.464133	-0.481895
H	6.857396	-2.879072	-1.317924
C	-5.567039	2.009308	1.444131
H	-5.929510	3.025090	1.238977
C	-5.240540	1.663240	2.872182
H	-4.425859	2.309144	3.235906
H	-6.111729	1.828740	3.524717
H	-4.926370	0.614655	2.962619
C	6.222563	1.247048	-0.038589
C	5.409436	1.847805	1.120114
H	5.922046	2.731262	1.531336
H	4.408677	2.164710	0.788419
H	5.289396	1.114484	1.932940
C	7.604983	0.826984	0.464776

H	8.205631	0.380754	-0.342120
H	8.147576	1.703164	0.851259
H	7.527636	0.087486	1.276084
C	6.369345	2.282758	-1.163559
H	6.884297	3.182100	-0.791320
H	6.953427	1.873490	-2.001754
H	5.386704	2.590152	-1.553061
C	-6.203930	-0.658261	-1.110466
C	-6.535716	-0.257538	-2.556701
H	-7.233405	-0.982388	-3.005015
H	-7.003283	0.738198	-2.591736
H	-5.627691	-0.229811	-3.178878
C	-7.474716	-0.645305	-0.258252
H	-8.209306	-1.356189	-0.666347
H	-7.256308	-0.934709	0.780738
H	-7.937914	0.352799	-0.242635
C	-5.583210	-2.064120	-1.089557
H	-6.311325	-2.804508	-1.455429
H	-4.699314	-2.116536	-1.743906
H	-5.275520	-2.349181	-0.072805
C	4.129265	0.227988	-1.076260
C	-3.852889	0.361009	-1.082509
C	5.957425	-3.379452	0.670572
H	5.545840	-4.329647	0.297650
H	6.865635	-3.619607	1.246026
H	5.216060	-2.924069	1.340162
C	0.817012	0.282514	1.619202
C	0.833049	-1.143554	1.554667
C	-0.473619	0.879459	1.658094
O	1.902204	1.003066	1.646007
C	-0.325304	-1.905813	1.502379
C	-1.630798	0.122538	1.637102
C	-1.546078	-1.260328	1.550431
H	2.673744	0.391753	1.588656
N	2.099915	-1.866800	1.547164
O	3.134913	-1.209013	1.629116
O	2.083577	-3.067308	1.478974
N	-0.654457	2.343891	1.721764
O	-1.797214	2.746397	1.788898
O	0.326163	3.045190	1.709890
N	-2.778323	-2.048008	1.488816
O	-2.687369	-3.201731	1.133044
O	-3.809015	-1.492901	1.803081
H	-2.597270	0.625233	1.660875
H	-0.263162	-2.989625	1.416600

$(MEA)_2A$:4

SCF = -2798.78086163

Num. Imaginary Freq = 0

C	-0.748002	2.424786	-2.601947
C	-1.377828	1.287155	-2.176914

C	-0.630969	0.187873	-1.654458	C	7.188341	-2.159152	-1.437312
C	0.790878	0.301048	-1.569986	H	7.569292	-2.032765	-2.459497
C	1.413105	1.505356	-2.019638	C	-6.324957	1.525169	-1.185905
C	0.666329	2.533876	-2.524851	H	-6.815813	1.706354	-2.151181
C	-1.269116	-0.999982	-1.202507	C	-6.256748	2.668974	-0.208662
C	1.554341	-0.772993	-1.036656	H	-5.805551	3.552405	-0.686271
C	0.924672	-1.994871	-0.681892	H	-7.265675	2.957299	0.126244
C	-0.497107	-2.112428	-0.774062	H	-5.651799	2.402286	0.668058
C	-1.113075	-3.337933	-0.387791	C	6.034664	0.905943	0.311077
H	-2.198722	-3.419225	-0.454201	C	5.567281	0.733405	1.765692
C	-0.361358	-4.385101	0.072682	H	5.864424	1.608834	2.364606
C	1.048689	-4.265356	0.174746	H	4.473871	0.639237	1.824564
C	1.674897	-3.104785	-0.192247	H	6.017895	-0.163427	2.217143
H	-1.334206	3.255635	-2.998832	C	7.560400	1.015361	0.264293
H	-2.464574	1.202468	-2.225899	H	7.923850	1.135080	-0.767869
H	2.498944	1.585947	-1.951362	H	7.889592	1.888759	0.847564
H	1.158154	3.446775	-2.865556	H	8.041097	0.122057	0.690670
H	-0.849541	-5.313645	0.373783	C	5.404825	2.171351	-0.291547
H	1.636492	-5.102690	0.555249	H	5.759690	3.061334	0.250915
H	2.757306	-3.004717	-0.105956	H	5.679677	2.284573	-1.352080
C	2.960303	-0.625733	-0.874896	H	4.308481	2.150465	-0.207890
C	-2.685968	-1.049083	-1.145732	C	-5.999250	-1.988710	0.034355
C	5.564489	-0.322931	-0.488808	C	-5.904953	-3.238519	-0.853881
C	-5.278159	-0.828139	-0.667965	H	-6.384100	-4.096315	-0.356873
C	-5.834783	0.336367	-0.952969	H	-6.406016	-3.076465	-1.820535
C	6.382639	-1.241991	-0.969597	H	-4.856338	-3.506423	-1.055262

C	-7.468087	-1.632310	0.272851	C	-1.768886	1.041739	1.336715
H	-7.980967	-2.469083	0.770908	C	-1.206855	2.366526	0.925560
H	-7.564216	-0.743608	0.914670	C	-0.781321	-0.004402	1.743934
H	-7.990530	-1.424904	-0.673496	O	-2.955053	0.833285	1.376900
C	-5.301329	-2.246884	1.379447	C	0.119098	2.614792	0.945320
H	-5.799264	-3.071269	1.913416	Cl	-2.363474	3.544286	0.477407
H	-4.243907	-2.519007	1.246674	C	0.558560	0.241927	1.758500
H	-5.332001	-1.350438	2.016272	C	-1.334813	-1.244654	2.189714
C	4.155746	-0.495167	-0.697193	C	1.110681	1.570459	1.352833
C	-3.885165	-0.968790	-0.959329	Cl	0.783956	4.138489	0.544536
C	7.637295	-3.379550	-0.679893	C	1.508709	-0.717149	2.229150
H	7.349521	-4.296002	-1.218356	N	-1.786900	-2.243957	2.557554
H	8.733960	-3.390810	-0.579788	O	2.294519	1.793102	1.383025
H	7.195222	-3.412606	0.324989	N	2.278119	-1.487092	2.621214